Spontaneous inhomogeneous phases in ultracold dipolar Fermi gases

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We study the collapse of ultracold fermionic gases into inhomogeneous states due to strong dipolar interaction in both 2D and 3D. Depending on the dimensionality, we find that two different types of inhomogeneous states are stabilized once the dipole moment reaches a critical value $d > d_c$: the *stripe phase* and *phase separation* between high and low densities. In 2D, we prove that the stripe phase is always favored for $d \gtrsim d_c$, regardless of the microscopic details of the system. In 3D, the one-loop perturbative calculation suggests that the same type of instability leads to phase separation. Experimental detection and finite-temperature effects are discussed.

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The rapid experimental development of ultracold atomic and molecular physics has opened up new opportunities to study quantum many-body systems with electric and magnetic dipolar interactions [1–9]. An important feature of dipolar interaction is its explicit spatial anisotropy of the $d_{r^2-3z^2}$-type when dipole moments are aligned by external fields. For the fermionic dipolar systems, ^{40}K-^{87}Rb has been cooled down almost to quantum-degeneracy [1]. Anisotropic Fermi liquid theories of the single particle and collective properties have been investigated [10–16]. Furthermore, unconventional Cooper pairing structures have been studied, including the p_z-channel pairing in the single component systems [17–22], and the competition between the $s+d$-wave singlet and the p_z-wave triplet channels [23–25]. In particular, a novel pairing state of the $s+ip$ type broken time-reversal symmetry has been pointed out [25]. Moreover, magnetic dipolar systems of fermions have also been experimentally realized [6]. Exotic states of the ferronematic Fermi liquid and unconventional magnetic states have been predicted [26, 27].

Fermionic systems can spontaneously break translational symmetry in both charge and spin channels. Many years ago, Overhauser pointed out that even in the weak coupling regime of the interacting electron gas, a $2k_f$ spin-density wave state always wins over the uniform paramagnetic state at the Hartree-Fock level [28]. However, correlation effects may suppress this instability and such a state has not been experimentally confirmed. Recently, quantum liquid crystal phases in strongly correlated systems have been intensively studied, particularly in doped Mott insulators [29]. Stripe ordering has been observed in high T_c cuprates, other transition metal oxides, and quantum Hall systems at high Landau levels [29–32].

In this article, we study the instability toward the spontaneous inhomogeneous phase in dipolar fermionic systems. In two dimensional (2D) systems, the strongest density-channel instability occurs at non-zero momentum, which drives the density wave states under strong dipolar interactions. This effect is based on the peculiar feature of the Fourier transform of the dipolar interaction, which is robust against microscopic details. However in three dimensions (3D), the instability at the one-loop level occurs at zero momentum, thus it leads to phase separation into high and low density regions.

We consider the single-component dipolar Fermi gas with dipole moment aligned by an external electric field. The long-distance physics of this system is described by the following Hamiltonian

$$H = \sum_{\vec{k}} (\epsilon_{\vec{k}} - \mu) c^\dagger_{\vec{k}} c_{\vec{k}} + \sum_{\vec{k},\vec{k}',\vec{q}} V(\vec{q}) c^\dagger_{\vec{k}+\vec{q}} c_{\vec{k}} c^\dagger_{\vec{k}'-\vec{q}} c_{\vec{k}'}, \quad (1)$$

with $\epsilon_{\vec{k}}$ being the energy dispersion relation and μ the chemical potential. In 2D, the dipolar interaction in the momentum space $V_{2\mathrm{D}}(\vec{q})$ takes the form [13],

$$V_{2\mathrm{D}}(\vec{q}) = 2\pi d^2 P_2(\cos\theta)[\frac{1}{\epsilon} - q] + \pi q d^2 \sin^2\theta \cos 2\phi_q, \quad (2)$$

where d is the dipole moment; ϕ_q is the azimuthal angle of the momentum $\vec{q}$ and θ is the angle between the direction of the dipoles and the z-axis. ϵ is a short-range cutoff roughly equal to the thickness of the system along the z-direction. Equation (2) is valid for $q\epsilon \ll 1$. However, as shown below, the main conclusion of this paper is independent of the value of $V(\vec{q})$ at large q. Equation (2) contains an isotropic part which depends on the microscopic cut-off ϵ and an anisotropic part which depends on the azimuthal angle of ϕ_q. We first consider the purely anisotropic case at $\theta = \theta_0 = \cos^{-1}\frac{1}{\sqrt{3}}$, and then the interaction simplifies into

$$V_{2\mathrm{D}}(\vec{q}) = \frac{2\pi d^2}{3} q \cos 2\phi_q. \quad (3)$$

The major feature of Eq. (3) is its linear dependence on q, which play important roles in driving the instability at non-zero wavevectors.

The stability of a system against density fluctuations is determined by the static susceptibility of density fluctuations:

$$\Pi_{2\mathrm{D}}(\vec{q}, \omega = 0) = \langle \rho(\vec{q}, \omega = 0) \rho(-\vec{q}, \omega = 0) \rangle, \quad (4)$$

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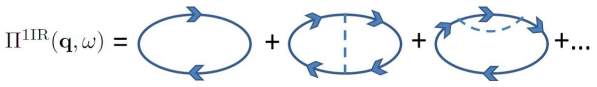

FIG. 1: (online color) Diagrammatic expansion for $\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q})$. The solid lines are free-fermion propagators and the dashed lines represent the dipolar interaction.

where $\rho(\vec{q},\omega) = \sum_{\vec{k},\Omega} c^{\dagger}_{\vec{k}+\vec{q},\Omega+\omega} c_{\vec{k},\Omega}$ is the density operator. The inverse of $\Pi_{2\mathrm{D}}(\vec{q},\omega=0)$ is the energy gap $\Delta_{2\mathrm{D}}(\vec{q})$ of creating a density wave at momentum $\vec{k}$. Using the technique of the diagrammatic expansion, $\Delta_{2\mathrm{D}}(\vec{q})$ can be computed order by order as

$$\begin{aligned}\Delta_{2\mathrm{D}}(\vec{q}) &= \Pi_{2\mathrm{D}}(\vec{q},\omega=0)^{-1} \\ &= [\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q},\omega=0)]^{-1} + V_{2\mathrm{D}}(\vec{q}), \end{aligned} \quad (5)$$

where $\Pi^{1\mathrm{IR}}(\vec{q},\omega)$ is the one-particle-irreducible density-density correlation [33, 34] shown in Fig. 1. The stability criteria of the homogeneous phase corresponds to the energy gap $\Delta_{2\mathrm{D}}(\vec{q})$ being positive-definite for any $\vec{q}$. Otherwise, the creation of a density wave could lower the total energy of the system leading to the condensation of density waves. Obviously, $\Delta_{2\mathrm{D}}(\vec{q})$ is positive-define for any $\vec{q}$ in the noninteracting Fermi gas. This stability remains for a weakly-interacting Fermi liquid. On the other hand, if the interaction has an attractive channel (e.g. the dipolar interaction in Eq. (3)), an inhomogeneous state could take advantage of the attractive interaction. Under strong enough attractive interactions, i.e., $V_{2\mathrm{D}} \to -\infty$, the homogeneous ground state is unstable.

We begin from the weak coupling side, by tuning up the interaction strength. In general, there is a critical dipole moment d_c such that $\Delta_{2\mathrm{D}}(\vec{q}) > 0$ at any $\vec{q}$ for $d < d_c$, but $\Delta_{2\mathrm{D}}(\vec{q}) < 0$ at some $\vec{q}$ for $d > d_c$. At $d = d_c$, $\Delta_{2\mathrm{D}}(\pm\vec{Q}) = 0$ for the momenta $\pm\vec{Q}$ and remain positive at other momenta [35]. If we increase d further above d_c, the density wave fluctuations with momentum $\vec{q} \sim \vec{Q}$ undergo an instability and condense. Depending on whether $\vec{Q}$ is 0 or not, this instability has two different fates. If $Q > 0$, the condensation carries a nonzero momentum, which leads to a stripe state: a unidirectional charge-density-wave state with wavevector $\vec{Q}$. On the other hand, if $\vec{Q} = 0$, the condensation takes place at an infinite wavelength and results in phase separation between high and low density regions. Here, the typical size of these high (low) density regions and their spatial arrangements are determined by the microscopic details of the system. In the particular case of a dipolar gas, the phase separation is sensitive to the details of the short-range behaviors of the interaction.

Due to the 2D space-inversion symmetry $\vec{r} \to -\vec{r}$, $[\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q},\omega)]^{-1}$ is an even function of $\vec{q}$. As a result, the Taylor expansion of $\Delta_{2\mathrm{D}}(\vec{q})$ at small momentum must

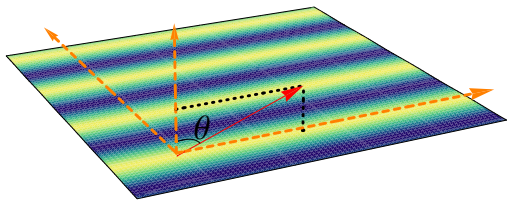

FIG. 2: (online color) The stripe phase in 2D dipolar gases. The three dotted arrows mark the x, y and z axes. The lighter (darker) regions in the 2D plane represent higher (lower) density. The solid line with an arrow represents the direction of the external field, which aligns the direction of the dipoles.

take the following form

$$\begin{aligned}\Delta_{2\mathrm{D}}(\vec{q}) =& [\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q}=0)]^{-1} + \frac{2\pi d^2}{3} q\cos 2\phi_q \\ &+ \frac{1}{2}\sum_{i,j} \partial_{q_i}\partial_{q_j}[\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q})]^{-1}|_{\vec{q}=0} q_i q_j + \ldots \end{aligned} \quad (6)$$

We focus on the most unstable direction $\phi_q = \frac{\pi}{2}$, in which the attraction in $V_{2\mathrm{D}}(\vec{q})$ is the strongest and the linear q term in Eq. (6) has a negative coefficient. Hence the point $\vec{q}=0$ is a local saddle point of $\Delta_{2\mathrm{D}}(\vec{q})$. Therefore, as d increases, $\Delta_{2\mathrm{D}}(\vec{q})$ at some finite momentum will become negative before $\Delta_{2\mathrm{D}}(\vec{q}=0)$ could reach zero. Thus, Q must be a nonzero value, which indicates that the system will collapse into a stripe phase for $d > d_c$, instead of phase separating. This is the main conclusion of this paper. It is noteworthy that this conclusion only depends on the small-momentum (i.e. long-range) behaviors of the interaction $V(\vec{q})$. Therefore, the stripe instability is a universal property of the 2D dipolar Fermi gas at $d > d_c$, insensitive to the microscopic details of the system.

More importantly, the conclusion of $Q > 0$ is a non-perturbative result which remains valid to any order in the loop expansion of Fig. 1. The only assumption required here is the analyticity of $\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q},\omega=0)$ as a function of $\vec{q}$ near $\vec{q}=0$. In a Fermi liquid, it is well-known that $\Pi^{1\mathrm{IR}}(\vec{q},\omega=0)$ is non-analytic at $\vec{q}=2k_F$ where k_F is the Fermi wavevector. However, there is no reason of a non-analytic behavior at small momentum in any Fermi liquid to our knowledge. The higher-order diagrams in Fig. 1 contain interaction lines which are non-analytic at small momenta. However, due to the fact that dipolar interactions are short-ranged in 2D, we do not expect any singularity for $\Pi^{1\mathrm{IR}}_{2\mathrm{D}}(\vec{q},\omega=0)$ around $\vec{q}=0$.

We check this conclusion using the loop expansion in Fig. 1 to the one-loop level for a continuum 2D system ($\epsilon_{\vec{k}} = k^2/2m$ with m being the mass of the particles) and find

$$\Delta_{2\mathrm{D}}(\vec{q}) = \frac{2\pi}{m}\left[\frac{1}{1-\sqrt{1-\frac{1}{x^2}}\eta(1-x)} + \frac{d^2}{d_c^2} x\cos 2\phi_{\vec{q}}\right], \quad (7)$$

where $x = \frac{q}{2k_F}$ and d_c is the critical dipole momentum

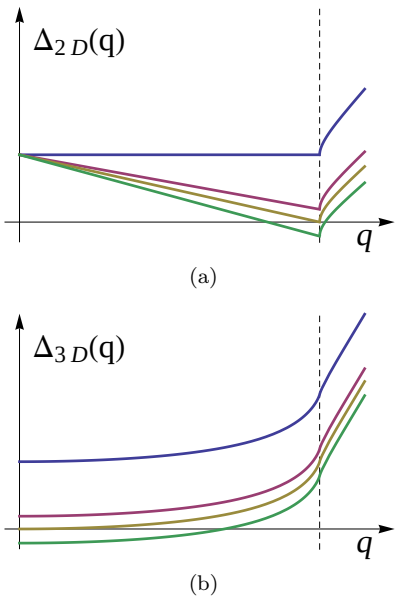

FIG. 3: (online color) One-loop calculation of $\Delta(\vec{q})$ in (a) $2D$ and (b) $3D$. In the $2D$ case, we choose $\phi_{\vec{q}} = \frac{\pi}{2}$ and for the $3D$, $\theta_{\vec{q}} = \pi/2$. From top to bottom, the dipole momentum for each of the curves are: $d/d_c = 0$, 0.9, 1, and 1.1 respectively. The dashed vertical line marks the momentum $2k_F$.

$d_c = \sqrt{\frac{3}{2k_F m}}$. $\phi_{\vec{q}}$ is the azimuthal angle of the momentum $\vec{q}$ and $\eta(x)$ is a step function with $\eta(x) = 1$ for $x > 0$ and $\eta(x) = 0$ for $x < 0$. As shown in Fig. 3(a), $Q = 2k_F$. If higher order corrections are considered, although the value of Q may vary, the fact that $Q > 0$ remains valid.

For $\theta \neq \theta_0$, the same conclusion applies for the single component case. The ϵ-term in Eq. (2) is momentum independent, which corresponds to short-range contact interaction. Thus it has no effect on the single component fermions, and $V(q) = q\pi d^2[-2P_2(\cos\theta) + \sin^2\theta\cos 2\phi_q]$. Along $\phi_q = \frac{\pi}{2}$ which remains the direction of the strongest instability, $V(q)$ is negative and grows linearly with q for an arbitrary value of θ, and the above conclusion still holds. We notice that even for $\theta = 0$, i.e., when the dipoles are perpendicular to the plane, the stripe instability still exists at large values of d although the interaction is now repulsive. For such an isotropic system (at $\theta = 0$), it is often assumed that three charge density waves form a triangular lattice to minimize the breaking of the rotational symmetry [36]. However, if the rotational symmetry is spontaneously broken before the homogeneous state becomes unstable, a stripe phase can be stabilized at zero temperature [37]. In this case, the stripe ordering spontaneously breaks both the rotational symmetry and the translational symmetry in the direction perpendicular to the stripes, while only the latter is spontaneously breaking in the stripe phases at $\theta \neq 0$. Due to its unique symmetry breaking pattern, the low-energy properties of the stripe phase at $\theta = 0$ is described by the quantum McMillan-de Gennes theory, which is fundamentally different from other similar phases at $\theta \neq 0$ [37]. Due to this unique property, the stripe phase at $\theta = 0$ is unstable at any finite temperature due to thermal fluctuations [37, 38], while the stripe phases at $\theta \neq 0$ has a power-law quasi-long range order blow a transition temperature T_{KT} (See below for details).

In 3D, the dipolar interaction is $V_{3D}(\vec{q}) = \frac{8\pi d^2}{3} P_2(\cos\theta_{\vec{q}})$, with θ_q measuring the angle between $\vec{q}$ and the dipole moment. Due to the structure of V_{3D}, the linear term of $\vec{q}$ in Eq. (6) is absent in 3D, and hence we could not exclude the possibility of $\vec{Q}$ being zero. In fact, the one-loop calculation for a system in continuum shows that

$$\Delta_{3D}(\vec{q}) = \frac{4\pi^2 k_F}{m}[(1 + \frac{1}{2x}(1-x^2)\log|\frac{1+x}{1-x}|)^{-1} + \frac{d^2}{d_C^2}(3\cos\theta_{\vec{q}}^2 - 1)], \quad (8)$$

where $x = q/2k_F$ and $d_c = \sqrt{3m/(32k_F\pi^3)}$. As can be seen from Fig. 3(b), $\vec{Q} = 0$, implying a phenomenon of phase separation for $d > d_c$. As discussed above, this is sensitive to the short-range details of the interaction and no universal conclusion is available for this phase separation.

Now we briefly discuss the multi-component case in 2D (e.g. the degrees of freedom of hyperfine spins). For simplicity we only consider the case of $N = 2$. In this case, the ϵ-term in Eq. (2) cannot be ignored, which naturally exists in the inter-component interactions. Following the same argument as in the single-component case studied above, the instability in the charge channel for a 2D system with $\theta > \theta_0$ leads to a charge stripe phase. However, for $\theta < \theta_0$ the short-range part becomes repulsive, so the density wave state is not favorable.

The stripe phase has a density modulation in the direction perpendicular to the stripes, which can be detected directly via the measurement of the local densities. In addition, any scattering experiments would show two interference Bragg peaks at momentum $\pm\vec{Q}$ in a stripe phase due to this density modulation. There are also other indirect tools to detect a stripe phase. Considering a density wave with density varying along the y axis [e.g. a density profile $\rho(x, y) = \rho_0 + \rho_1\cos(Qy + \phi)$ with (x, y) being the 2D coordinate in the real space], if we place this system in a shallow potential trap and then introduce an extra narrow 1D potential well along the direction of the stripe [e.g. $V(x, y) = \alpha y^2$], it is energetically favorable to have $y = 0$ being a high density region due to the potential well $V(x, y)$. If we move the potential trap along the y direction but keep the location of the potential well $V(x, y)$ unchanged, the stripes will largely remain at their initial positions if the displacement of the trap is less than half the wave-length of the stripes $\pi/\vec{Q}$, and the stripes will jump over a distance of $2\pi/\vec{Q}$ if the displacement becomes larger than $\pi/\vec{Q}$. On the other hand, the jump

would not happen in a homogeneous state. This jump will lead to a center of mass oscillation for the trapped particles due to the lack of dissipation, which could serve as an indirect signature for the stripe phase.

Since a real system has a finite temperature, the contribution of the thermal fluctuations comes into play. Their effects can be studied based on the symmetry-breaking pattern of the ordered phase. For a 2D system in the continuum, the homogeneous phase at $d < d_C$ has continuous translational and two-fold rotational symmetries (rotation by π) at $\theta \neq 0$. For $d > d_C$, the stripe phase spontaneously breaks the continuous translational symmetry in one direction and leads to one gapless Goldstone mode as required by symmetry. In a 2D system with $d > d_C$, if we increase the temperature from $T = 0$, such a Goldstone mode will destroy the long-range order of the stripe phase. However, a quasi-long-range power-law correlation would still remain for temperature below a transition temperature $T_{\rm KT}$ [38]. For $T < T_{\rm KT}$, although the real-space density oscillation of the stripes is hard to observe due to the lack of a true long-range order, the density profile in Fourier space will have two peaks located at $\pm\vec{Q}$ which decays as a power-law function of $|\vec{q}\mp\vec{Q}|$. Above $T_{\rm KT}$, the correlation becomes short-ranged and the phase transition at $T = T_{\rm KT}$ belongs to the usual Kosterlitz−Thouless (KT) university class.

For dipolar molecules in a 2D optical lattice, if the wavevector of the stripe phase is commensurate with the lattice wavevector, the stripe phase breaks no continuous symmetry and hence no gapless Goldstone mode is present. Therefore, the long-range order of the stripe phase remains at finite T below a critical temperature T_C. However, if the stripe phase is incommensurate with the underlying lattice, the KT physics described above is expected.

In summary, we find that the 2D dipolar Fermi gas undergoes a stripe ordering at large dipolar interaction strength, i.e., the density wave instability at finite momentum, instead of phase separation. For the single component case, this instability occurs regardless of the dipole orientation. This arises from the fact that the Fourier transform of the dipolar interaction increases linearly with wavevector. For the multicomponent case, due to the short-range Hartree interaction, the stripe instability only exists at $\theta > \theta_0$.

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